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Structural and elastic properties of zinc-blende and wurtzite InN_{1-x}Bi_x alloys

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Abstract

Structural and elastic properties of InN_{1-x}Bi_x alloys in both zinc-blende and wurtzite phases are studied by using first-principle calculations. Two different Bi-atom arrangements of uniform and clustered configurations have been considered for $x=0.25$, 0.5 , and 0.75 . It is found that clustered configuration has a significant effect on lattice parameters of wurtzite InN_{1-x}Bi_x alloys. A slightly sublinear dependence on the alloy content, x , can be accepted for C_{11} , C_{12} , C_{13} , and C_{33} in zinc-blende InN_{1-x}Bi_x, and for C_{12} , C_{13} , and C_{44} in wurtzite InN_{1-x}Bi_x, whereas clearly linear deviations are obtained for C_{44} and C_{66} in zinc-blende alloys and for C_{11} and C_{33} in wurtzite alloys. The effect of Bi atoms clustering leads to a decrease in all elastic constants and bulk modulus in zinc-blende InN_{1-x}Bi_x, and makes big deviations from Vegard's-like law and has little influence on bulk modulus in wurtzite InN_{1-x}Bi_x alloys.

Keywords: zinc-blende; wurtzite; clustered arrangement; InN_{1-x}Bi_x; elastic constant.

1. Introduction

The group-III nitrides have been the focus of intensive concern because of their

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